Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.05

Global applicability domain: Inside

Local applicability domain index: 7.12e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

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Fenitrooxone
Measured: 1.69
Predicted: 2.05

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Paraoxon
Measured: 1.98
Predicted: 2.18

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Phosphoric acid, dimethyl 3,5-dimethyl-4-nitrophenyl ester
Measured: 2.57
Predicted: 2.23